



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:03 am GMT

PDB ID : 3NCY
Title : X-ray crystal structure of an arginine agmatine antiporter (AdiC) in complex with a Fab fragment
Authors : Fang, Y.; Jayaram, H.; Shane, T.; Komalkova-Partensky, L.; Wu, F.; Williams, C.; Xiong, Y.; Miller, C.
Deposited on : 2010-06-06
Resolution : 3.20 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

<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

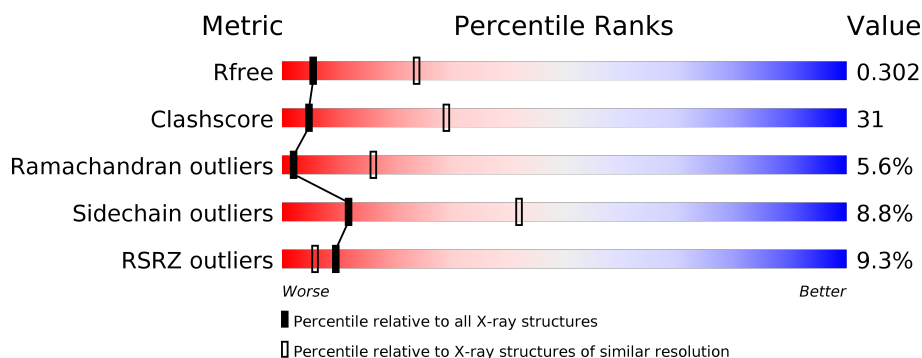
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	445	<div> <div>12%</div> <div> <div>47%</div> <div>40%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	445	<div> <div>8%</div> <div> <div>46%</div> <div>40%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	445	<div> <div>7%</div> <div> <div>47%</div> <div>41%</div> <div>7%</div> <div>6%</div> </div> </div>
1	D	445	<div> <div>9%</div> <div> <div>47%</div> <div>41%</div> <div>7%</div> <div>6%</div> </div> </div>
2	P	219	<div> <div>5%</div> <div> <div>46%</div> <div>45%</div> <div>9%</div> </div> </div>
2	Q	219	<div> <div>12%</div> <div> <div>46%</div> <div>46%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	S	211	<div><div></div><div>4%</div><div>58%</div><div>36%</div><div>6%</div></div>
3	W	211	<div><div></div><div>13%</div><div>57%</div><div>36%</div><div>7%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18693 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 AdiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3052	2018	489	524	21			
1	B	420	Total	C	N	O	S	5	0	0
			3039	2009	489	520	21			
1	C	420	Total	C	N	O	S	0	0	0
			3034	2006	487	520	21			
1	D	419	Total	C	N	O	S	17	0	0
			3031	2005	486	519	21			

- Molecule 2 is a protein called Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	218	Total	C	N	O	S	16	0	0
			1640	1044	264	325	7			
2	P	219	Total	C	N	O	S	15	0	0
			1647	1049	265	326	7			

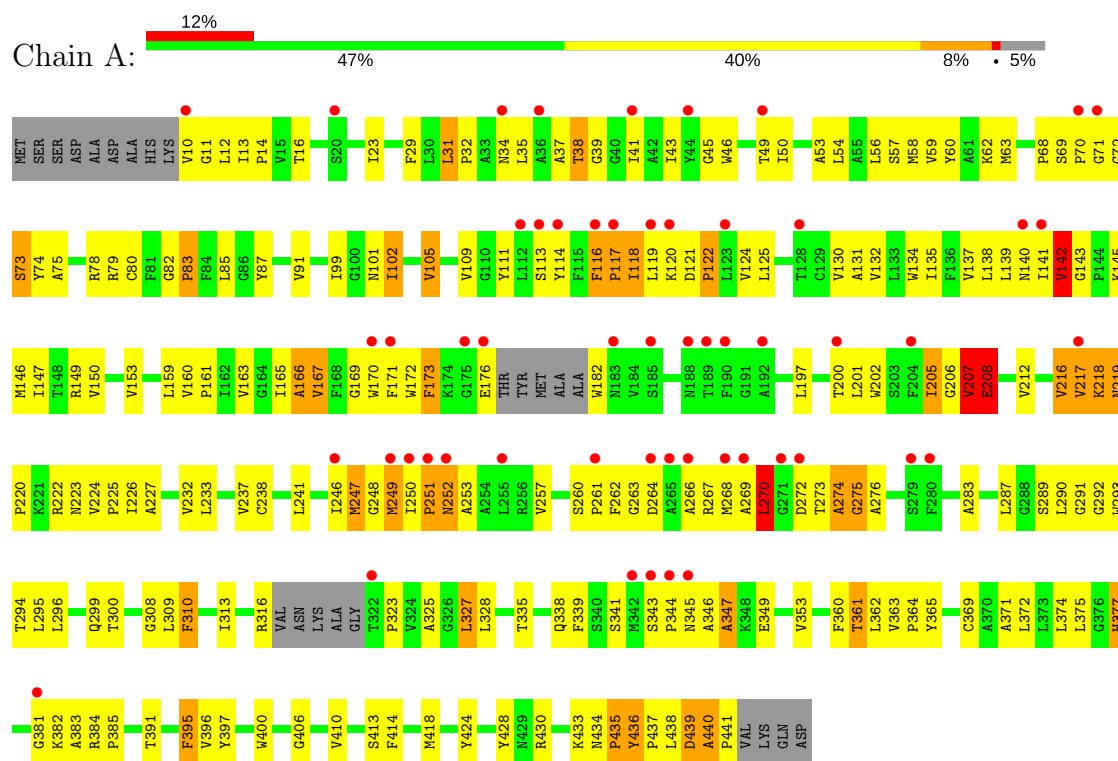
- Molecule 3 is a protein called Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	211	Total	C	N	O	S	40	0	0
			1625	1011	271	333	10			
3	S	211	Total	C	N	O	S	20	0	0
			1625	1011	271	333	10			

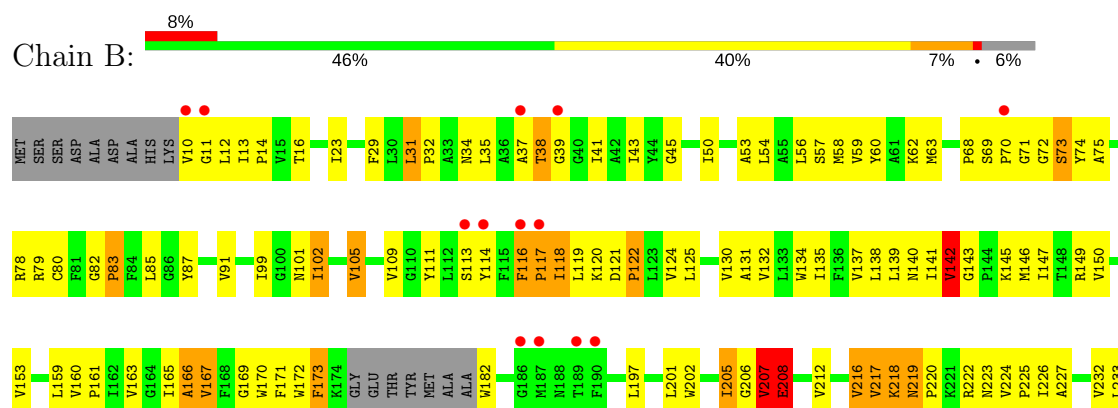
3 Residue-property plots

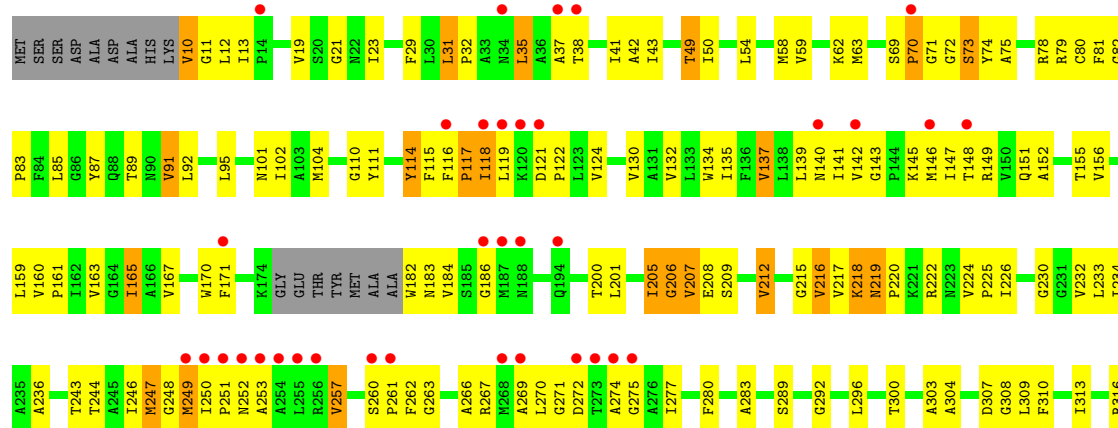
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($RSRZ > 2$). 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.

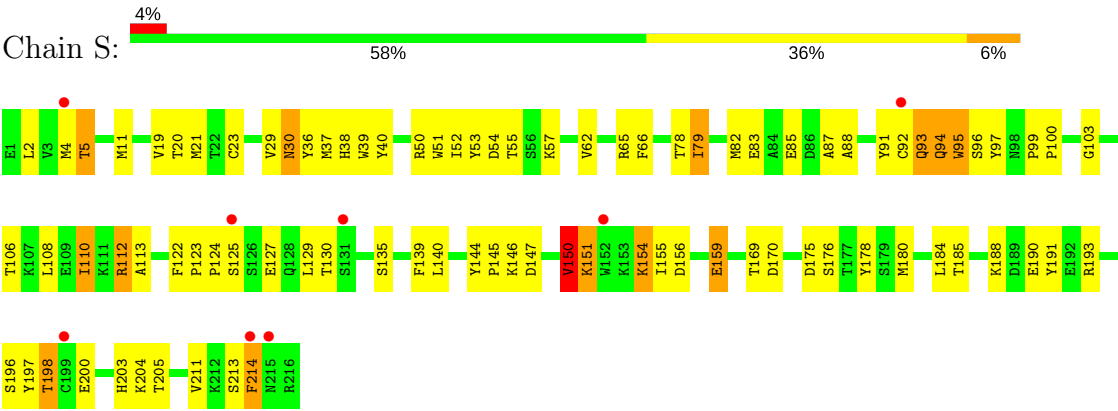
• Molecule 1: AdiC



• Molecule 1: AdiC







4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.66Å 104.15Å 154.03Å 81.96° 75.93° 73.73°	Depositor
Resolution (Å)	33.23 – 3.20 45.88 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.4 (33.23-3.20) 94.1 (45.88-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.282 , 0.312 0.274 , 0.302	Depositor DCC
R_{free} test set	3612 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 84.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	18693	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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 [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	0.22	0/3125	0.42	0/4281
1	B	0.22	0/3110	0.43	0/4257
1	C	0.22	0/3107	0.43	0/4256
1	D	0.22	0/3103	0.42	0/4250
2	P	0.22	0/1694	0.46	1/2319 (0.0%)
2	Q	0.23	0/1686	0.46	0/2307
3	S	0.23	0/1665	0.42	0/2260
3	W	0.23	0/1665	0.43	0/2260
All	All	0.22	0/19155	0.43	1/26190 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	134	VAL	N-CA-C	-5.71	95.58	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	3052	0	3120	201	0
1	B	3039	0	3112	191	0
1	C	3034	0	3098	190	0
1	D	3031	0	3102	199	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1647	0	1601	128	0
2	Q	1640	0	1594	135	0
3	S	1625	0	1550	83	0
3	W	1625	0	1550	85	0
All	All	18693	0	18727	1142	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 31.

The worst 5 of 1142 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:346:ALA:HA	1:A:347:ALA:CB	1.58	1.24
1:A:346:ALA:CA	1:A:347:ALA:HB3	1.76	1.12
1:A:23:ILE:HG12	1:A:206:GLY:HA3	1.33	1.11
1:D:356:VAL:HG11	1:D:409:GLU:HB3	1.30	1.10
1:B:23:ILE:HG12	1:B:206:GLY:HA3	1.32	1.08

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	416/445 (94%)	328 (79%)	59 (14%)	29 (7%)	1	9
1	B	414/445 (93%)	328 (79%)	57 (14%)	29 (7%)	1	9
1	C	414/445 (93%)	322 (78%)	68 (16%)	24 (6%)	2	15
1	D	413/445 (93%)	319 (77%)	71 (17%)	23 (6%)	2	16
2	P	217/219 (99%)	179 (82%)	27 (12%)	11 (5%)	2	18
2	Q	216/219 (99%)	180 (83%)	25 (12%)	11 (5%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S	209/211 (99%)	174 (83%)	28 (13%)	7 (3%)	4	29
3	W	209/211 (99%)	173 (83%)	29 (14%)	7 (3%)	4	29
All	All	2508/2640 (95%)	2003 (80%)	364 (14%)	141 (6%)	2	16

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	PHE
1	A	118	ILE
1	A	166	ALA
1	A	270	LEU
1	A	274	ALA

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	308/343 (90%)	280 (91%)	28 (9%)	11	39
1	B	306/343 (89%)	277 (90%)	29 (10%)	10	37
1	C	305/343 (89%)	286 (94%)	19 (6%)	21	60
1	D	306/343 (89%)	286 (94%)	20 (6%)	20	58
2	P	187/187 (100%)	166 (89%)	21 (11%)	7	29
2	Q	186/187 (100%)	162 (87%)	24 (13%)	5	22
3	S	185/185 (100%)	169 (91%)	16 (9%)	12	43
3	W	185/185 (100%)	168 (91%)	17 (9%)	11	38
All	All	1968/2116 (93%)	1794 (91%)	174 (9%)	12	42

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	35	LEU
2	Q	6	GLN

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Mol	Chain	Res	Type
3	S	79	ILE
1	D	114	TYR
1	D	316	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	299	GLN
1	C	434	ASN
3	W	94	GLN
1	B	377	HIS
3	W	30	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 [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	422/445 (94%)	0.68	55 (13%) 4 2	56, 127, 231, 339	0
1	B	419/445 (94%)	0.39	35 (8%) 12 7	62, 126, 220, 332	0
1	C	420/445 (94%)	0.30	30 (7%) 17 10	37, 105, 203, 283	0
1	D	416/445 (93%)	0.49	40 (9%) 9 5	33, 105, 197, 283	0
2	P	218/219 (99%)	0.44	12 (5%) 26 15	48, 104, 168, 282	2 (0%)
2	Q	216/219 (98%)	0.67	27 (12%) 4 3	44, 108, 171, 278	2 (0%)
3	S	209/211 (99%)	0.31	8 (3%) 41 27	30, 80, 169, 258	0
3	W	207/211 (98%)	0.55	28 (13%) 3 2	23, 81, 166, 266	0
All	All	2527/2640 (95%)	0.48	235 (9%) 9 6	23, 109, 203, 339	4 (0%)

The worst 5 of 235 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	135	CYS	21.8
1	D	250	ILE	12.5
2	Q	137	ASP	11.9
1	B	264	ASP	8.2
1	B	117	PRO	7.7

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.