



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:44 PM GMT

PDB ID : 5E6P
Title : PlexinB2 cytoplasmic region/PDZ-RhoGEF PDZ domain complex
Authors : Pascoe, H.G.; Zhang, X.
Deposited on : 2015-10-10
Resolution : 3.21 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

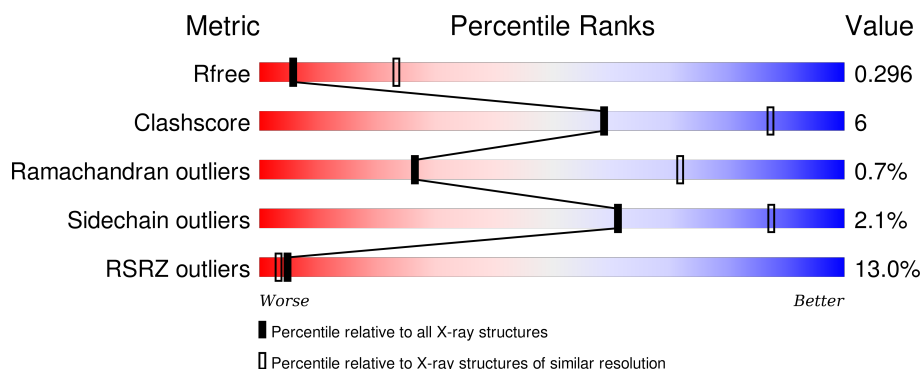
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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	621	
2	B	88	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4478 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 Plexin-B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	504	3946	2550	652	727	17	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1222	GLY	-	expression tag	UNP B2RXS4
A	1223	PRO	-	expression tag	UNP B2RXS4
A	1224	HIS	-	expression tag	UNP B2RXS4
A	1225	MET	-	expression tag	UNP B2RXS4

- Molecule 2 is a protein called Rho guanine nucleotide exchange factor 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	75	532	337	95	97	3	0	0	0

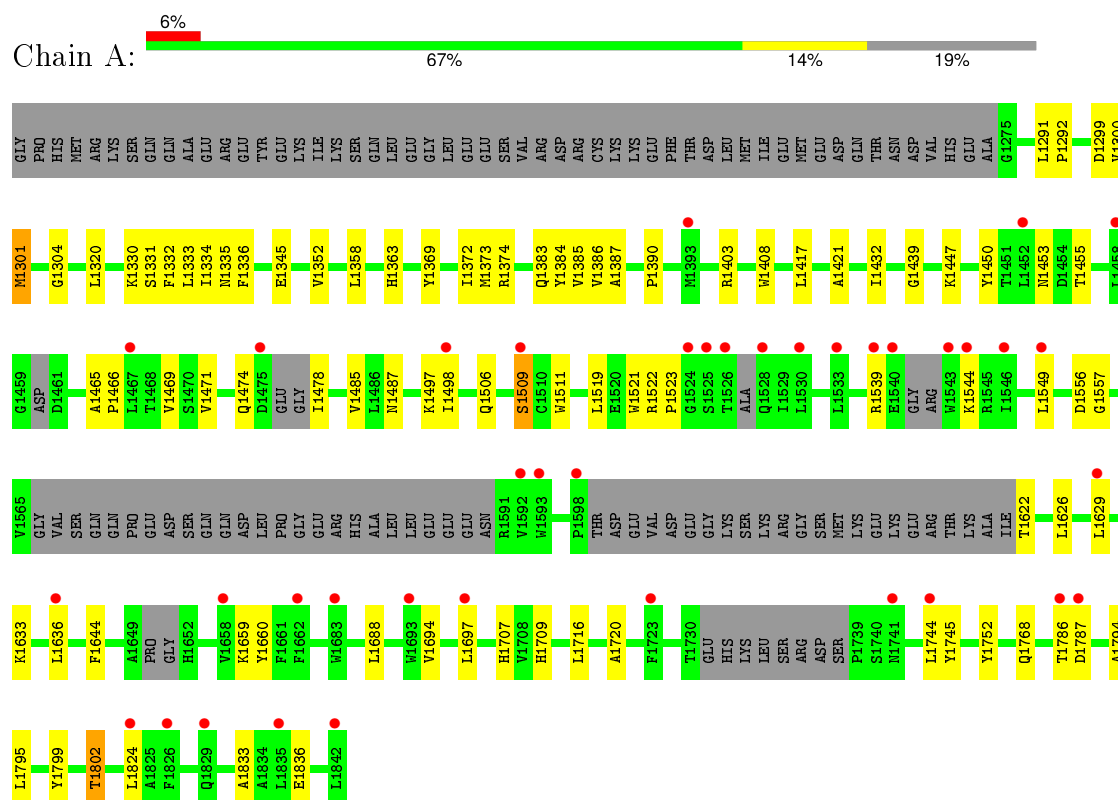
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	38	GLY	-	expression tag	UNP O15085
B	39	PRO	-	expression tag	UNP O15085
B	40	HIS	-	expression tag	UNP O15085
B	41	MET	-	expression tag	UNP O15085

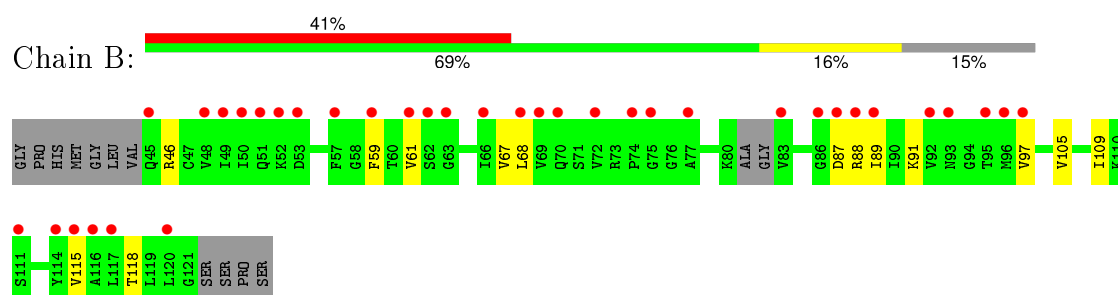
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Plexin-B2



• Molecule 2: Rho guanine nucleotide exchange factor 11



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	126.15Å 126.15Å 211.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.53 – 3.21 48.53 – 3.22	Depositor EDS
% Data completeness (in resolution range)	86.3 (48.53-3.21) 82.9 (48.53-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.254 , 0.297 0.253 , 0.296	Depositor DCC
R_{free} test set	731 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	130.6	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 86.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 16810 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4478	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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

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	0.26	0/4027	0.43	0/5480
2	B	0.30	0/536	0.47	0/724
All	All	0.27	0/4563	0.43	0/6204

There are no bond length outliers.

There are no bond angle outliers.

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	3946	0	3839	43	1
2	B	532	0	538	9	0
All	All	4478	0	4377	51	1

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.

All (51) 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:1417:LEU:HA	1:A:1421:ALA:HB3	1.73	0.69
2:B:91:LYS:HB3	2:B:118:THR:HB	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1352:VAL:HA	1:A:1403:ARG:HG2	1.76	0.68
2:B:67:VAL:HG11	2:B:105:VAL:HG11	1.80	0.62
1:A:1374:ARG:NH2	1:A:1660:TYR:OH	2.32	0.62
1:A:1332:PHE:HB2	1:A:1824:LEU:HD13	1.81	0.62
1:A:1506:GLN:O	1:A:1511:TRP:NE1	2.33	0.60
1:A:1629:LEU:HB3	1:A:1744:LEU:HD21	1.84	0.59
1:A:1539:ARG:HG2	1:A:1544:LYS:HA	1.85	0.58
1:A:1556:ASP:OD1	1:A:1557:GLY:N	2.41	0.54
1:A:1521:TRP:O	1:A:1523:PRO:HD3	2.10	0.52
2:B:59:PHE:HE2	2:B:61:VAL:HG23	1.75	0.51
1:A:1432:ILE:HG12	1:A:1636:LEU:HD13	1.93	0.50
1:A:1659:LYS:HZ2	1:A:1768:GLN:HA	1.78	0.48
1:A:1474:GLN:HA	1:A:1478:ILE:HG12	1.95	0.48
1:A:1453:ASN:OD1	1:A:1455:THR:OG1	2.26	0.48
1:A:1659:LYS:NZ	1:A:1768:GLN:HA	2.29	0.48
1:A:1622:THR:O	1:A:1626:LEU:HG	2.14	0.47
1:A:1694:VAL:HG13	1:A:1720:ALA:HB1	1.95	0.47
1:A:1301:MET:HE3	1:A:1794:ALA:HB2	1.97	0.47
1:A:1333:LEU:HD23	1:A:1372:ILE:HG13	1.96	0.46
2:B:89:ILE:HG22	2:B:97:VAL:HG21	1.97	0.46
1:A:1369:TYR:CE1	1:A:1373:MET:HE3	2.51	0.46
1:A:1363:HIS:HB3	1:A:1786:THR:HG22	1.98	0.46
1:A:1300:VAL:O	1:A:1304:GLY:N	2.48	0.46
1:A:1352:VAL:HG13	1:A:1403:ARG:NE	2.31	0.45
2:B:109:ILE:HG23	2:B:115:VAL:HG21	1.98	0.45
1:A:1633:LYS:HG3	1:A:1745:TYR:CE2	2.52	0.45
1:A:1485:VAL:HG12	1:A:1497:LYS:HD3	1.98	0.45
1:A:1336:PHE:CZ	1:A:1802:THR:HG22	2.51	0.45
1:A:1301:MET:CE	1:A:1794:ALA:HB2	2.46	0.45
1:A:1383:GLN:O	1:A:1387:ALA:HB2	2.17	0.44
1:A:1373:MET:HE1	1:A:1408:TRP:HB2	1.98	0.44
1:A:1320:LEU:HD22	1:A:1795:LEU:HB3	1.99	0.44
1:A:1833:ALA:HA	2:B:68:LEU:CD1	2.48	0.44
1:A:1331:SER:O	1:A:1335:ASN:ND2	2.51	0.43
1:A:1299:ASP:CG	1:A:1300:VAL:H	2.22	0.43
1:A:1799:TYR:OH	1:A:1836:GLU:OE2	2.36	0.43
2:B:59:PHE:CE2	2:B:61:VAL:HG23	2.53	0.43
1:A:1465:ALA:HA	1:A:1466:PRO:HD3	1.93	0.42
2:B:68:LEU:HB3	2:B:88:ARG:HA	2.01	0.42
1:A:1487:ASN:HA	1:A:1549:LEU:HB2	2.01	0.42
1:A:1385:VAL:HA	1:A:1390:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ARG:NH2	2:B:87:ASP:OD2	2.52	0.42
1:A:1707:HIS:O	1:A:1707:HIS:ND1	2.53	0.42
1:A:1330:LYS:HE3	1:A:1334:ILE:HD11	2.03	0.41
1:A:1447:LYS:NZ	1:A:1455:THR:O	2.54	0.41
1:A:1644:PHE:HD2	1:A:1752:TYR:CZ	2.39	0.41
1:A:1439:GLY:HA3	1:A:1450:TYR:CD1	2.57	0.40
1:A:1697:LEU:O	1:A:1716:LEU:HB3	2.21	0.40
1:A:1471:VAL:HG11	1:A:1498:ILE:HG21	2.02	0.40

All (1) 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:1509:SER:OG	1:A:1787:ASP:OD1[12_545]	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	486/621 (78%)	451 (93%)	31 (6%)	4 (1%)	24	69
2	B	71/88 (81%)	62 (87%)	9 (13%)	0	100	100
All	All	557/709 (79%)	513 (92%)	40 (7%)	4 (1%)	26	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1345	GLU
1	A	1688	LEU
1	A	1292	PRO
1	A	1386	VAL

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	419/564 (74%)	409 (98%)	10 (2%)	57	86
2	B	55/71 (78%)	55 (100%)	0	100	100
All	All	474/635 (75%)	464 (98%)	10 (2%)	61	87

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

Mol	Chain	Res	Type
1	A	1291	LEU
1	A	1301	MET
1	A	1358	LEU
1	A	1384	TYR
1	A	1469	VAL
1	A	1509	SER
1	A	1519	LEU
1	A	1522	ARG
1	A	1709	HIS
1	A	1802	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no ligands in this entry.

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 ⓘ

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	504/621 (81%)	0.52	39 (7%) 16 10	75, 135, 176, 203	0
2	B	75/88 (85%)	2.14	36 (48%) 0 0	129, 175, 204, 209	0
All	All	579/709 (81%)	0.73	75 (12%) 5 3	75, 139, 188, 209	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	83	VAL	8.6
1	A	1475	ASP	6.8
1	A	1741	ASN	6.7
2	B	48	VAL	6.0
2	B	50	ILE	5.8
1	A	1592	VAL	5.5
2	B	63	GLY	5.2
2	B	117	LEU	5.1
1	A	1543	TRP	5.0
1	A	1598	PRO	4.9
2	B	59	PHE	4.5
2	B	57	PHE	4.2
2	B	66	ILE	4.2
2	B	86	GLY	4.2
2	B	95	THR	4.2
2	B	49	ILE	3.9
1	A	1526	THR	3.9
2	B	45	GLN	3.9
2	B	89	ILE	3.7
1	A	1842	LEU	3.7
2	B	111	SER	3.6
2	B	92	VAL	3.5
2	B	114	TYR	3.4
2	B	61	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1636	LEU	3.3
1	A	1683	TRP	3.3
1	A	1744	LEU	3.3
1	A	1524	GLY	3.2
1	A	1540	GLU	3.1
2	B	120	LEU	3.1
2	B	72	VAL	3.0
2	B	97	VAL	2.9
2	B	116	ALA	2.9
1	A	1697	LEU	2.9
1	A	1544	LYS	2.8
1	A	1498	ILE	2.8
2	B	52	LYS	2.8
1	A	1393	MET	2.8
2	B	77	ALA	2.7
2	B	74	PRO	2.7
1	A	1452	LEU	2.7
2	B	93	ASN	2.6
2	B	69	VAL	2.6
1	A	1629	LEU	2.6
1	A	1693	TRP	2.6
2	B	62	SER	2.6
1	A	1662	PHE	2.5
1	A	1549	LEU	2.4
2	B	70	GLN	2.4
2	B	88	ARG	2.4
1	A	1826	PHE	2.4
1	A	1509	SER	2.4
1	A	1525	SER	2.4
2	B	51	GLN	2.4
1	A	1546	ILE	2.3
2	B	87	ASP	2.3
1	A	1829	GLN	2.3
1	A	1528	GLN	2.3
1	A	1658	VAL	2.3
1	A	1723	PHE	2.3
2	B	96	MET	2.3
1	A	1787	ASP	2.3
2	B	53	ASP	2.3
1	A	1533	LEU	2.2
1	A	1539	ARG	2.2
2	B	115	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1458	LEU	2.2
1	A	1824	LEU	2.2
1	A	1835	LEU	2.1
1	A	1467	LEU	2.1
2	B	68	LEU	2.1
1	A	1530	LEU	2.1
2	B	75	GLY	2.1
1	A	1593	TRP	2.0
1	A	1786	THR	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.