



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:10 PM GMT

PDB ID : 4HGM
Title : Shark IgNAR Variable Domain
Authors : Olland, A; Kovalenko, O.V.; King, D.; Svenson, K.
Deposited on : 2012-10-08
Resolution : 2.34 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

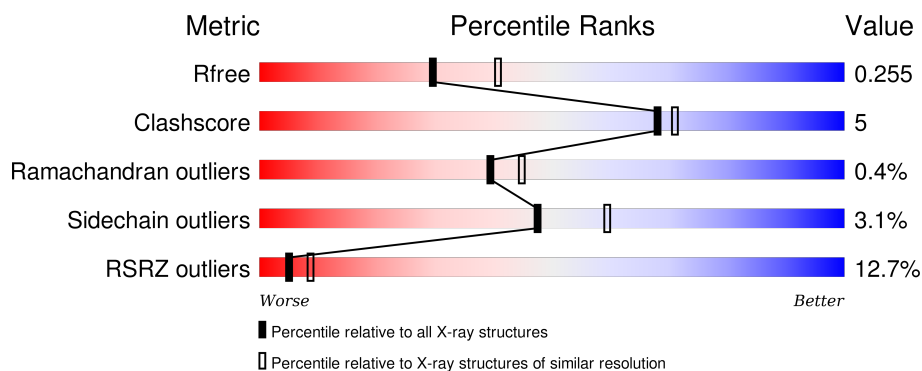
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.34 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	112	 79% 13% • 8%
2	B	585	 13% 71% 10% • 18%

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
4	ACE	B	602	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4577 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 Shark V-NAR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			791	494	130	164	3			

- Molecule 2 is a protein called Serum albumin.

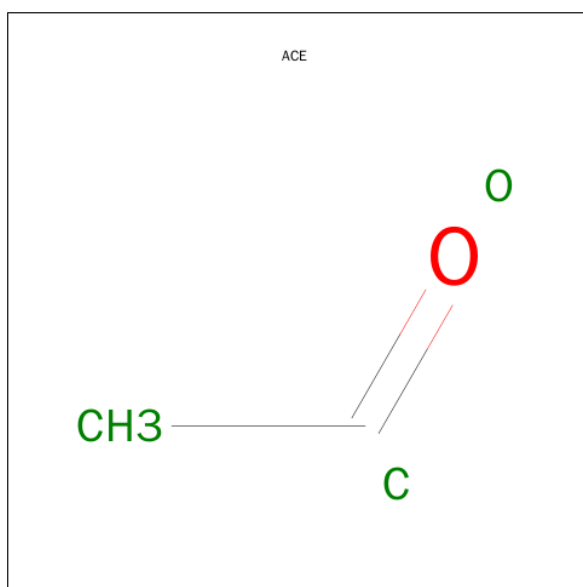
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	478	Total	C	N	O	S	0	0	0
			3707	2342	632	697	36			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ACETYL GROUP (three-letter code: ACE) (formula: C₂H₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			3	2	1		


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	50	Total	O	0	0
			50	50		

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.

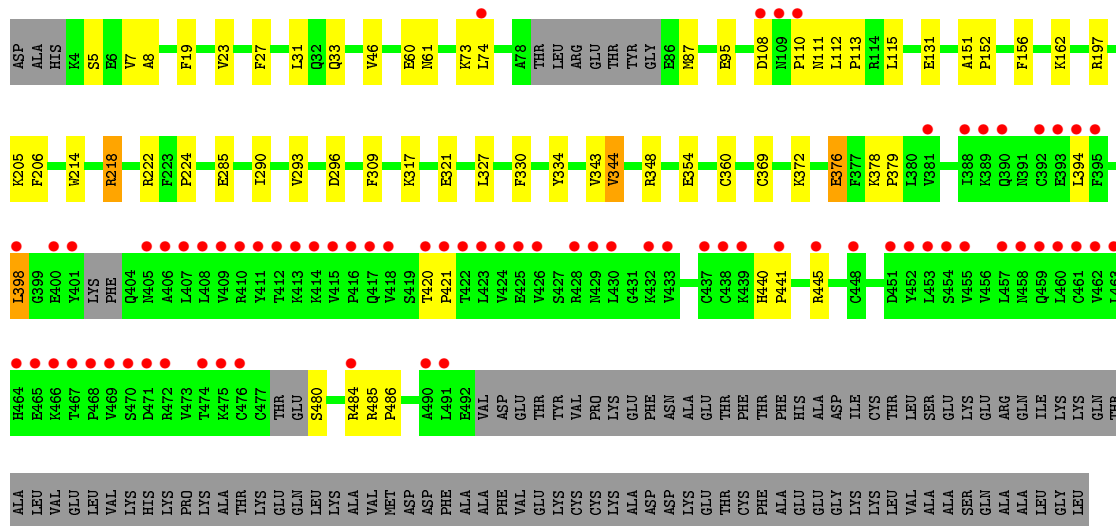
• Molecule 1: Shark V-NAR

Chain A: 



• Molecule 2: Serum albumin

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.34Å 131.34Å 74.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.91 – 2.34 65.67 – 2.34	Depositor EDS
% Data completeness (in resolution range)	95.4 (37.91-2.34) 99.5 (65.67-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.221 , 0.259 0.217 , 0.255	Depositor DCC
R_{free} test set	3048 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.7	EDS
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 31462 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4577	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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

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

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	0.31	0/807	0.50	0/1096
2	B	0.27	0/3779	0.41	0/5111
All	All	0.27	0/4586	0.43	0/6207

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	791	0	766	8	0
2	B	3707	0	3546	33	0
3	B	4	0	6	0	0
4	B	3	0	3	0	0
5	A	22	0	0	0	0
5	B	50	0	0	0	0
All	All	4577	0	4321	41	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 5.

All (41) 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)
2:B:485:ARG:HB3	2:B:486:PRO:HD3	1.70	0.73
2:B:317:LYS:HE2	2:B:321:GLU:OE2	2.04	0.57
2:B:378:LYS:HB2	2:B:379:PRO:HD3	1.86	0.56
1:A:89:ASN:O	1:A:90:ILE:HG22	2.06	0.56
2:B:222:ARG:C	2:B:224:PRO:HD3	2.28	0.53
2:B:112:LEU:HB3	2:B:113:PRO:HD2	1.90	0.53
2:B:156:PHE:CE1	2:B:285:GLU:HB3	2.45	0.52
1:A:76:GLU:H	1:A:76:GLU:CD	2.14	0.51
2:B:344:VAL:O	2:B:348:ARG:HG3	2.10	0.51
2:B:224:PRO:HD2	2:B:296:ASP:HB3	1.93	0.51
2:B:376:GLU:O	2:B:379:PRO:HD2	2.12	0.49
2:B:327:LEU:HD11	2:B:354:GLU:HG3	1.94	0.49
2:B:480:SER:O	2:B:484:ARG:HG3	2.13	0.49
2:B:441:PRO:O	2:B:445:ARG:HG3	2.13	0.49
1:A:11:SER:HA	1:A:101:GLU:O	2.12	0.49
2:B:5:SER:HB3	2:B:8:ALA:HB3	1.95	0.48
2:B:420:THR:N	2:B:421:PRO:HD2	2.28	0.48
2:B:372:LYS:HE2	2:B:372:LYS:HA	1.96	0.47
2:B:394:LEU:O	2:B:398:LEU:HB2	2.14	0.47
2:B:218:ARG:HD3	2:B:218:ARG:O	2.14	0.47
2:B:214:TRP:CD1	2:B:343:VAL:HG11	2.49	0.46
1:A:29:TYR:CD1	1:A:89:ASN:HB3	2.51	0.46
2:B:60:GLU:O	2:B:61:ASN:HB2	2.17	0.45
2:B:31:LEU:HD22	2:B:74:LEU:HD22	1.99	0.45
1:A:36:TRP:CZ3	1:A:83:CYS:HB3	2.52	0.45
2:B:156:PHE:HE1	2:B:285:GLU:HB3	1.81	0.45
2:B:290:ILE:O	2:B:293:VAL:HG12	2.18	0.44
1:A:42:GLY:O	1:A:43:SER:HB2	2.18	0.44
2:B:46:VAL:HG23	2:B:73:LYS:HG2	2.00	0.43
2:B:218:ARG:C	2:B:218:ARG:HD3	2.38	0.43
2:B:440:HIS:HB3	2:B:441:PRO:HD2	2.00	0.43
2:B:309:PHE:CZ	2:B:330:PHE:HA	2.54	0.43
1:A:1:THR:HG23	1:A:27:THR:HB	2.00	0.43
1:A:39:GLN:HG2	1:A:43:SER:HA	2.00	0.42
2:B:115:LEU:HA	2:B:115:LEU:HD23	1.93	0.42
2:B:27:PHE:CD1	2:B:74:LEU:HD21	2.55	0.41
2:B:151:ALA:N	2:B:152:PRO:HD2	2.36	0.41
2:B:19:PHE:O	2:B:23:VAL:HG23	2.21	0.41
2:B:360:CYS:HB3	2:B:369:CYS:HB3	1.93	0.40
2:B:205:LYS:HB3	2:B:206:PHE:HD2	1.86	0.40
2:B:131:GLU:OE2	2:B:162:LYS:HE3	2.21	0.40

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	101/112 (90%)	97 (96%)	3 (3%)	1 (1%)	19	18
2	B	470/585 (80%)	447 (95%)	22 (5%)	1 (0%)	52	61
All	All	571/697 (82%)	544 (95%)	25 (4%)	2 (0%)	39	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ILE
2	B	110	PRO

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	90/97 (93%)	87 (97%)	3 (3%)	45	57
2	B	392/511 (77%)	380 (97%)	12 (3%)	47	59
All	All	482/608 (79%)	467 (97%)	15 (3%)	47	59

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG

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Mol	Chain	Res	Type
1	A	18	VAL
1	A	90	ILE
2	B	7	VAL
2	B	33	GLN
2	B	87	MET
2	B	95	GLU
2	B	108	ASP
2	B	111	ASN
2	B	197	ARG
2	B	218	ARG
2	B	334	TYR
2	B	344	VAL
2	B	376	GLU
2	B	398	LEU

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 [i](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
3	EDO	B	601	-	3,3,3	0.38	0	2,2,2	0.53	0
4	ACE	B	602	-	2,2,2	0.62	0	0,1,1	0.00	-

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
3	EDO	B	601	-	-	0/1/1/1	0/0/0/0
4	ACE	B	602	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	103/112 (91%)	0.22	0	100 100	32, 47, 65, 80	0
2	B	478/585 (81%)	0.91	74 (15%)	3 5	33, 58, 155, 173	0
All	All	581/697 (83%)	0.79	74 (12%)	5 9	32, 55, 152, 173	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	460	LEU	10.1
2	B	415	VAL	9.6
2	B	109	ASN	9.3
2	B	468	PRO	8.5
2	B	411	TYR	8.5
2	B	457	LEU	8.4
2	B	474	THR	7.7
2	B	418	VAL	7.6
2	B	410	ARG	7.5
2	B	405	ASN	7.4
2	B	401	TYR	7.3
2	B	465	GLU	7.0
2	B	462	VAL	6.7
2	B	470	SER	6.6
2	B	423	LEU	6.4
2	B	472	ARG	6.3
2	B	464	HIS	6.3
2	B	432	LYS	6.0
2	B	424	VAL	6.0
2	B	467	THR	6.0
2	B	463	LEU	5.9
2	B	400	GLU	5.6
2	B	414	LYS	5.6
2	B	455	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	416	PRO	5.0
2	B	458	ASN	4.9
2	B	421	PRO	4.8
2	B	466	LYS	4.7
2	B	395	PHE	4.6
2	B	406	ALA	4.6
2	B	445	ARG	4.5
2	B	413	LYS	4.3
2	B	408	LEU	4.2
2	B	412	THR	4.0
2	B	389	LYS	3.9
2	B	429	ASN	3.9
2	B	407	LEU	3.8
2	B	491	LEU	3.8
2	B	453	LEU	3.6
2	B	459	GLN	3.5
2	B	430	LEU	3.5
2	B	394	LEU	3.5
2	B	425	GLU	3.4
2	B	417	GLN	3.4
2	B	110	PRO	3.4
2	B	392	CYS	3.4
2	B	420	THR	3.4
2	B	461	CYS	3.2
2	B	437	CYS	3.2
2	B	422	THR	3.2
2	B	393	GLU	3.2
2	B	451	ASP	3.1
2	B	398	LEU	3.0
2	B	469	VAL	2.9
2	B	452	TYR	2.8
2	B	438	CYS	2.8
2	B	476	CYS	2.8
2	B	439	LYS	2.7
2	B	433	VAL	2.6
2	B	454	SER	2.6
2	B	409	VAL	2.6
2	B	390	GLN	2.5
2	B	448	CYS	2.5
2	B	471	ASP	2.5
2	B	484	ARG	2.3
2	B	381	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	490	ALA	2.3
2	B	426	VAL	2.2
2	B	428	ARG	2.2
2	B	74	LEU	2.1
2	B	108	ASP	2.1
2	B	441	PRO	2.1
2	B	475	LYS	2.0
2	B	388	ILE	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	ACE	B	602	3/3	0.89	0.22	3.32	46,46,48,52	0
3	EDO	B	601	4/4	0.85	0.17	1.37	55,56,59,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.