



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:53 AM UTC

PDB ID : 4LSG / pdb_00004lsg
Title : Structure of Mouse P-Glycoprotein
Authors : Chang, G.; Szewczyk, P.
Deposited on : 2013-07-22
Resolution : 3.80 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
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

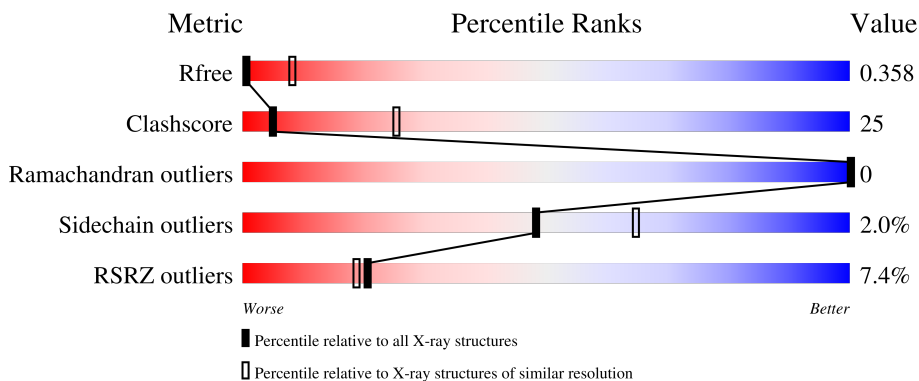
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	1284	 8% 51% 39% • 8%
1	B	1284	 6% 53% 38% • 8%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18352 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 Multidrug resistance protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1182	9170	5895	1552	1686	37	0	0	0
1	B	1182	9170	5895	1552	1686	37	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	952	ALA	CYS	engineered mutation	UNP P21447
A	1277	LEU	-	expression tag	UNP P21447
A	1278	GLU	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447
A	1283	HIS	-	expression tag	UNP P21447
A	1284	HIS	-	expression tag	UNP P21447
B	952	ALA	CYS	engineered mutation	UNP P21447
B	1277	LEU	-	expression tag	UNP P21447
B	1278	GLU	-	expression tag	UNP P21447
B	1279	HIS	-	expression tag	UNP P21447
B	1280	HIS	-	expression tag	UNP P21447
B	1281	HIS	-	expression tag	UNP P21447
B	1282	HIS	-	expression tag	UNP P21447
B	1283	HIS	-	expression tag	UNP P21447
B	1284	HIS	-	expression tag	UNP P21447

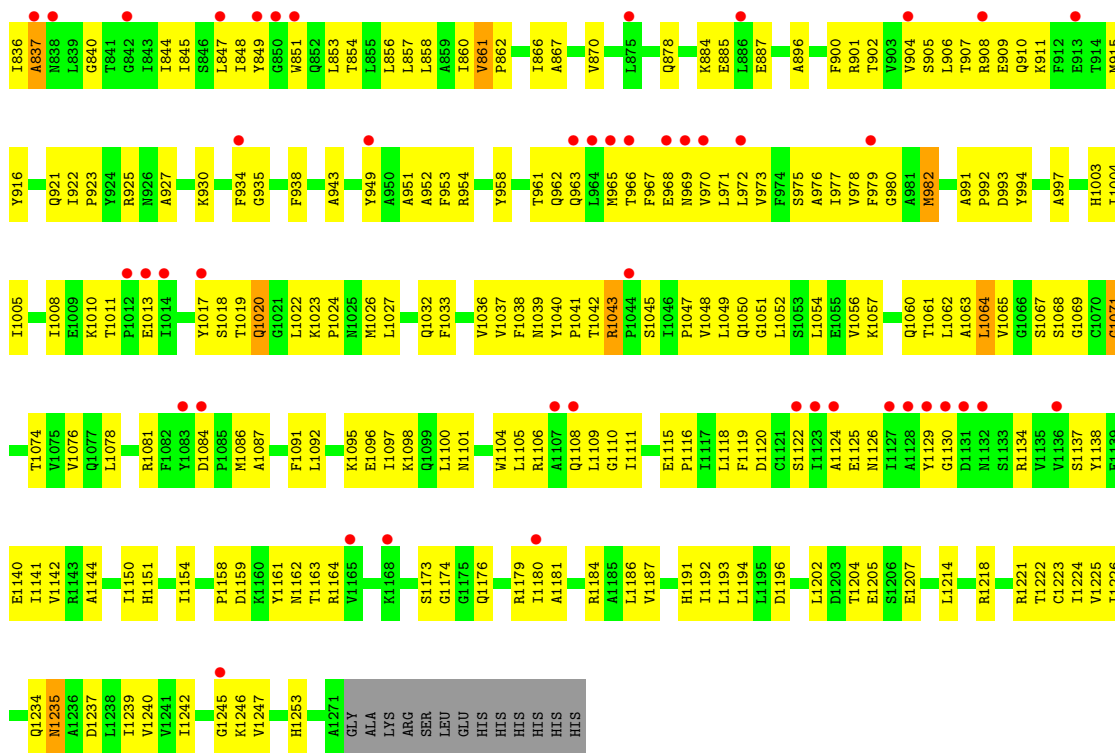
- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Hg	0	0
			6	6		

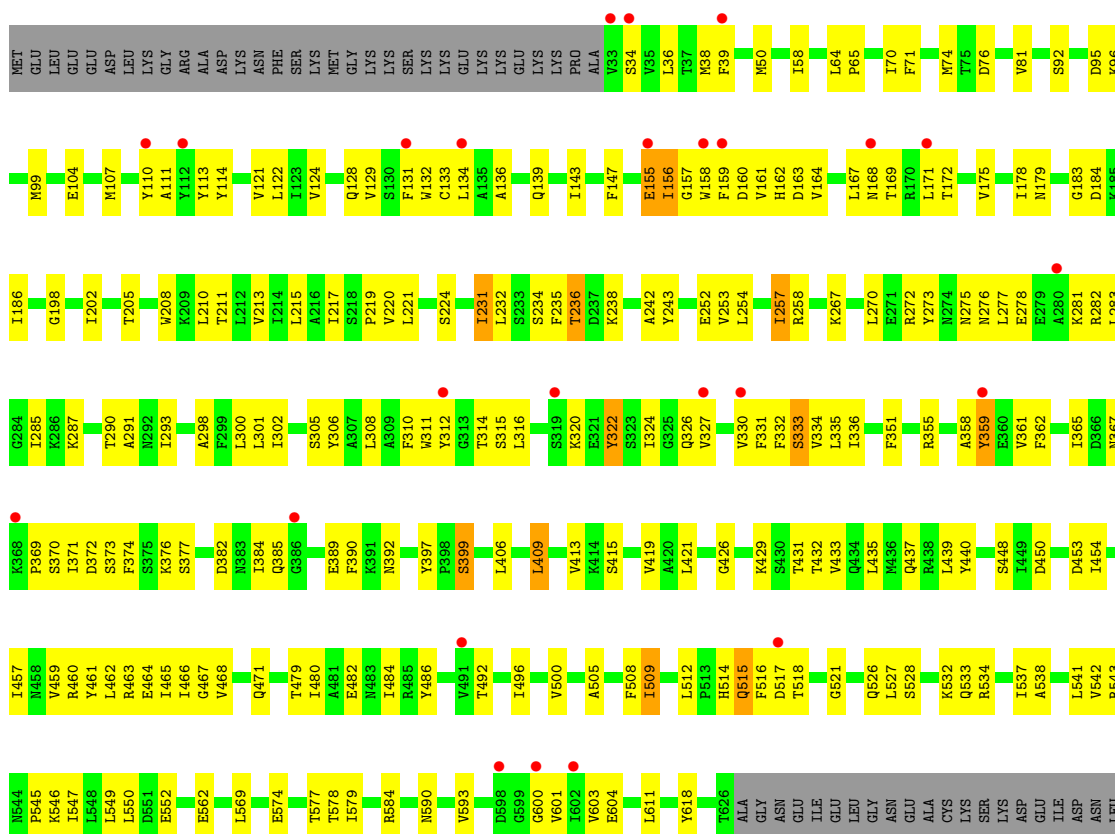
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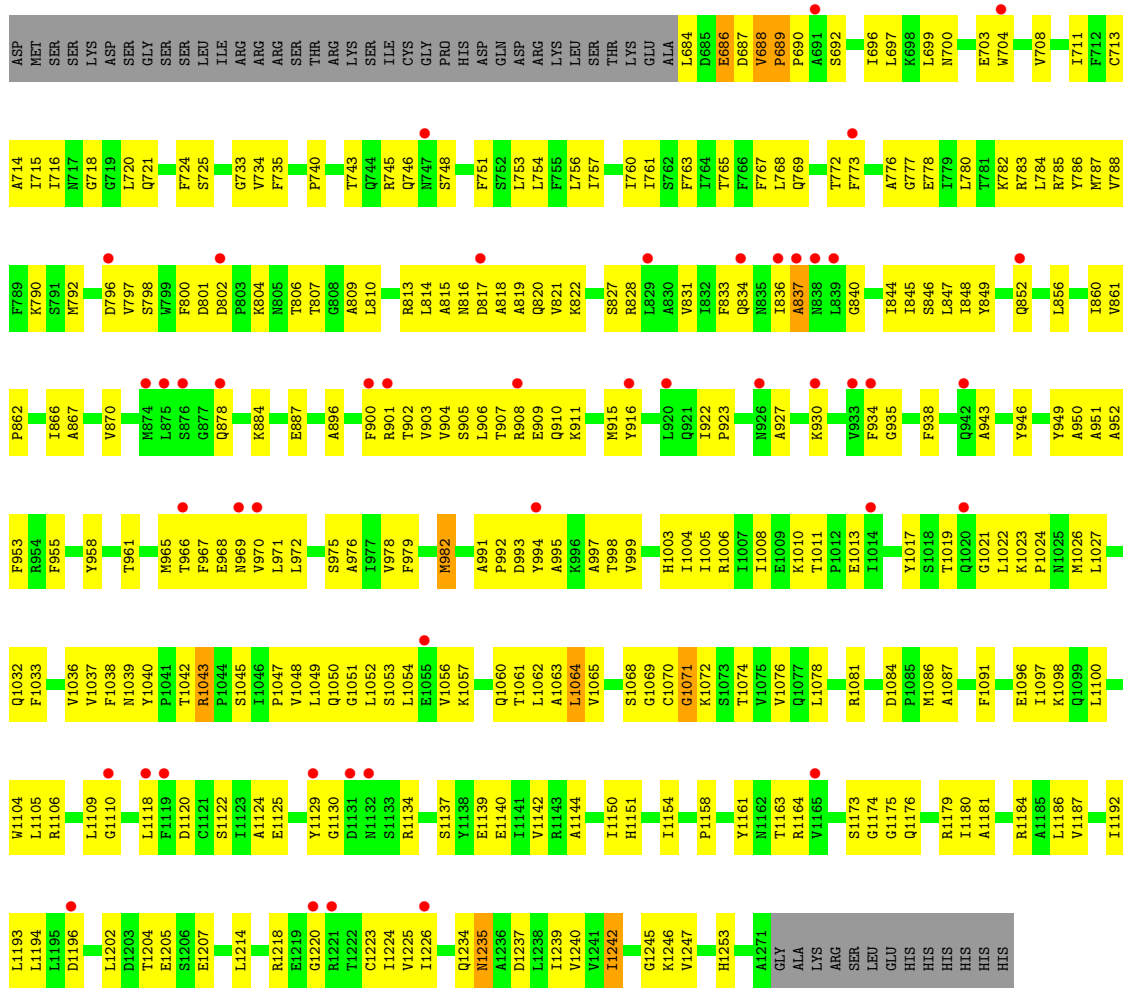
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total	Hg	0	0
			6	6		



● Molecule 1: Multidrug resistance protein 1A





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.54Å 115.43Å 378.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.80 19.98 – 3.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (19.98-3.80) 95.3 (19.98-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.69 (at 3.82Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.336 , 0.357 0.336 , 0.358	Depositor DCC
R_{free} test set	4203 reflections (9.73%)	wwPDB-VP
Wilson B-factor (Å ²)	133.9	Xtrriage
Anisotropy	0.338	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 15.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	18352	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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](#)

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

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	0.45	2/9338 (0.0%)	1.03	34/12625 (0.3%)
1	B	0.45	2/9338 (0.0%)	1.03	38/12625 (0.3%)
All	All	0.45	4/18676 (0.0%)	1.03	72/25250 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	688	VAL	C-N	6.41	1.41	1.33
1	B	688	VAL	C-N	6.26	1.40	1.33
1	B	689	PRO	N-CD	5.33	1.55	1.47
1	A	689	PRO	N-CD	5.29	1.55	1.47

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ILE	N-CA-C	9.10	119.02	110.74
1	B	231	ILE	N-CA-C	8.95	118.88	110.74
1	A	372	ASP	N-CA-C	-8.72	102.00	114.12
1	B	1043	ARG	CA-C-N	-7.35	114.23	121.65
1	B	1043	ARG	C-N-CA	-7.35	114.23	121.65

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	9170	0	9338	476	0
1	B	9170	0	9338	456	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
All	All	18352	0	18676	926	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 25.

The worst 5 of 926 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:B:132:TRP:CD1	1:B:183:GLY:HA3	1.53	1.42
1:A:1019:THR:CG2	1:A:1101:ASN:HA	1.50	1.41
1:A:107:MET:HE3	1:A:958:TYR:CD2	1.57	1.40
1:A:132:TRP:CD1	1:A:183:GLY:HA3	1.59	1.36
1:B:1017:TYR:CE2	1:B:1019:THR:HG23	1.65	1.30

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	1178/1284 (92%)	1069 (91%)	109 (9%)	0	100	100
1	B	1178/1284 (92%)	1069 (91%)	109 (9%)	0	100	100
All	All	2356/2568 (92%)	2138 (91%)	218 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	975/1064 (92%)	955 (98%)	20 (2%)	47 64
1	B	975/1064 (92%)	956 (98%)	19 (2%)	50 66
All	All	1950/2128 (92%)	1911 (98%)	39 (2%)	48 65

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	601	VAL
1	B	1225	VAL
1	B	743	THR
1	B	1064	LEU
1	B	1242	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1253	HIS
1	B	1114	GLN
1	B	154	GLN
1	B	942	GLN
1	B	128	GLN

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 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

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 [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	1182/1284 (92%)	0.59	105 (8%) 15 16	48, 98, 147, 186	0
1	B	1182/1284 (92%)	0.51	71 (6%) 27 22	50, 103, 148, 189	0
All	All	2364/2568 (92%)	0.55	176 (7%) 20 19	48, 100, 147, 189	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	823	GLY	8.1
1	A	312	TYR	6.8
1	A	749	ASN	6.4
1	A	1123	ILE	6.0
1	A	1083	TYR	5.7

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 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(\AA^2)	Q<0.9
2	HG	B	1302	1/1	-0.17	0.38	109,109,109,109	1
2	HG	A	1302	1/1	0.81	0.22	166,166,166,166	1
2	HG	A	1306	1/1	0.84	0.08	146,146,146,146	0
2	HG	A	1304	1/1	0.85	0.15	146,146,146,146	0
2	HG	B	1301	1/1	0.88	0.07	146,146,146,146	0
2	HG	A	1303	1/1	0.91	0.08	146,146,146,146	0
2	HG	B	1306	1/1	0.91	0.05	146,146,146,146	0
2	HG	B	1303	1/1	0.92	0.06	146,146,146,146	0
2	HG	A	1301	1/1	0.92	0.06	146,146,146,146	0
2	HG	B	1304	1/1	0.94	0.18	146,146,146,146	0
2	HG	A	1305	1/1	0.96	0.03	146,146,146,146	0
2	HG	B	1305	1/1	0.99	0.04	146,146,146,146	0

6.5 Other polymers [i](#)

There are no such residues in this entry.