



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 08:13 PM UTC

PDB ID : 2WIU / pdb_00002wiu
Title : Mercury-modified bacterial persistence regulator hipBA
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Fisher, D.A.
Deposited on : 2009-05-17
Resolution : 2.35 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
Xtrriage (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

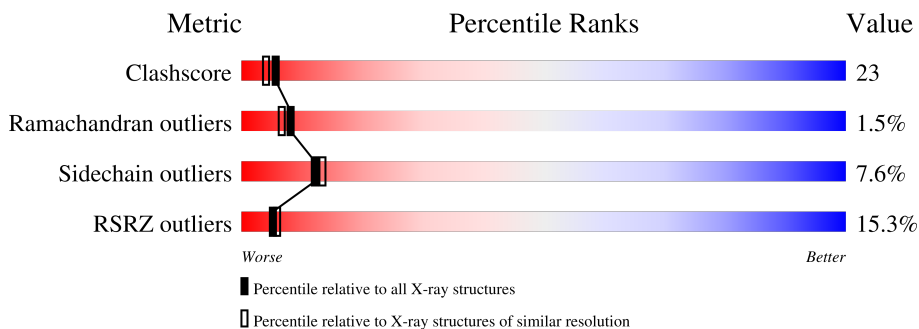
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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))
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	446	 17% (Poor fit), 61% (0 outliers), 28% (1 outlier), 6% (2 outliers), 8% (3+ outliers)
1	C	446	 13% (Poor fit), 54% (0 outliers), 31% (1 outlier), 10% (2 outliers), 8% (3+ outliers)
2	B	88	 8% (Poor fit), 47% (0 outliers), 32% (1 outlier), 19% (2 outliers), 10% (3+ outliers)
2	D	88	 10% (Poor fit), 48% (0 outliers), 24% (1 outlier), 9% (2 outliers), 19% (3+ outliers)

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8029 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 PROTEIN HIPA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	431	3397	2171	593	620	13	0	0	0
1	C	401	3190	2043	557	576	14	0	3	0

- Molecule 2 is a protein called HTH-TYPE TRANSCRIPTIONAL REGULATOR HIPB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	71	576	366	96	111	3	0	1	0
2	D	71	571	362	95	111	3	0	0	0

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Hg 2	0	0
3	B	1	Total 1	Hg 1	0	0
3	C	3	Total 3	Hg 3	0	0
3	D	1	Total 1	Hg 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	Cl 3	0	0
4	B	2	Total 2	Cl 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total 3	Cl 3	0	0
4	D	2	Total 2	Cl 2	0	0

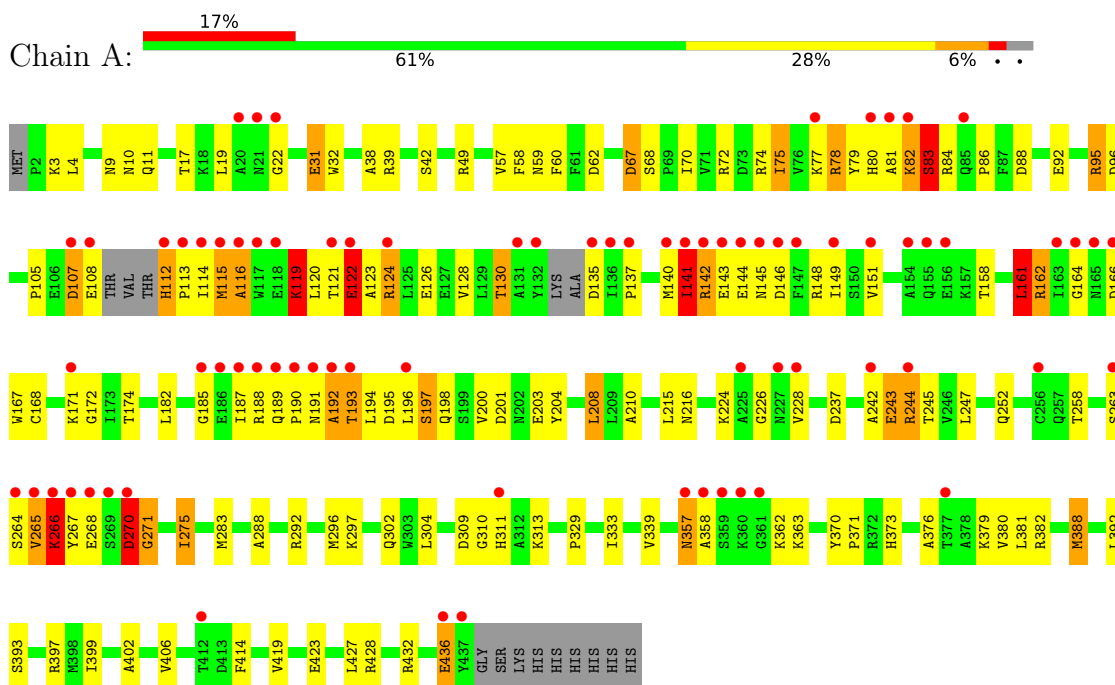
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total 108	O 108	0	0
5	B	18	Total 18	O 18	0	0
5	C	135	Total 135	O 135	0	0
5	D	17	Total 17	O 17	0	0

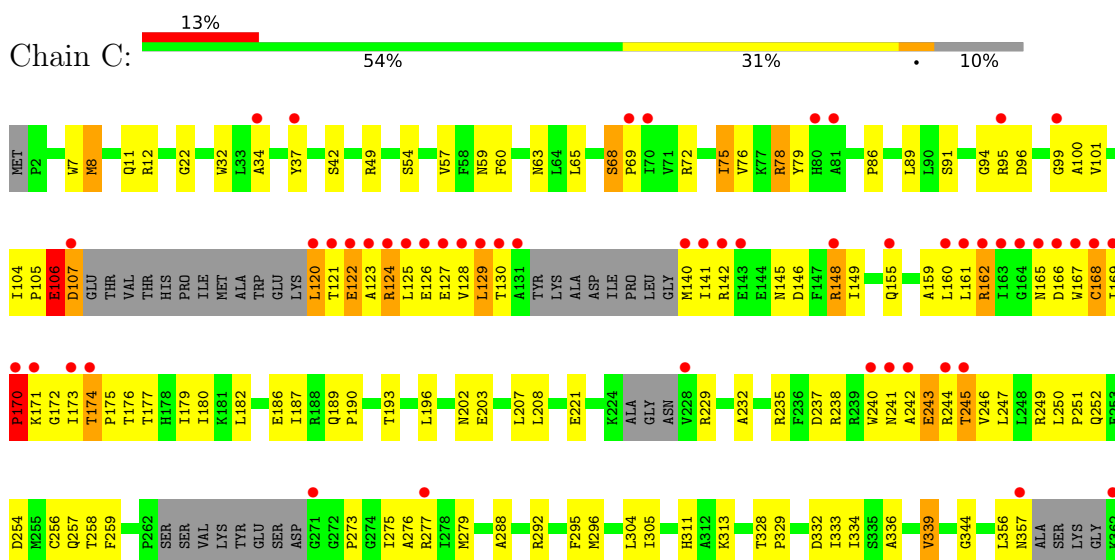
3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: PROTEIN HIPA

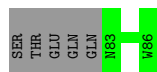
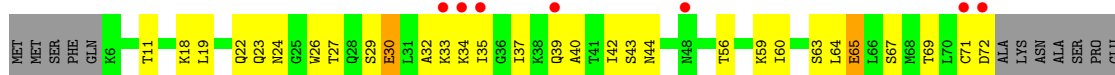


- Molecule 1: PROTEIN HIPA

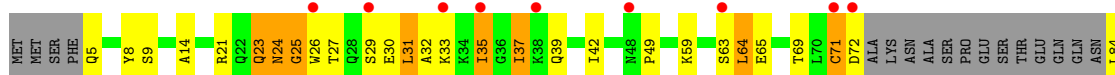




● Molecule 2: HTH-TYPE TRANSCRIPTIONAL REGULATOR HIPB



● Molecule 2: HTH-TYPE TRANSCRIPTIONAL REGULATOR HIPB



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	166.93Å 166.93Å 124.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	166.67 – 2.35 166.67 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (166.67-2.35) 88.8 (166.67-2.35)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.216 , 0.264 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtrriage
Anisotropy	0.377	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8029	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2189e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, 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	1.17	5/3470 (0.1%)	1.39	39/4701 (0.8%)
1	C	1.12	4/3264 (0.1%)	1.30	20/4418 (0.5%)
2	B	1.28	2/587 (0.3%)	1.19	3/790 (0.4%)
2	D	1.37	1/579 (0.2%)	1.30	3/780 (0.4%)
All	All	1.18	12/7900 (0.2%)	1.33	65/10689 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	4
2	B	0	1
2	D	0	2
All	All	0	11

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	LEU	C-N	-30.53	0.91	1.33
2	B	33	LYS	CG-CD	6.47	1.71	1.52
2	D	9	SER	C-O	-5.78	1.18	1.24
1	A	357	ASN	CG-OD1	5.78	1.34	1.23
1	C	344	GLY	C-O	-5.71	1.17	1.24

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	LEU	O-C-N	-14.89	103.83	123.19
1	A	161	LEU	CA-C-N	12.25	144.93	121.54
1	A	161	LEU	C-N-CA	12.25	144.93	121.54
1	A	162	ARG	CA-C-N	10.91	138.11	123.06
1	A	162	ARG	C-N-CA	10.91	138.11	123.06

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ASP	Peptide
1	A	164	GLY	Peptide
1	A	270	ASP	Peptide
1	A	358	ALA	Peptide
2	B	71	CYS	Peptide

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	3397	0	3426	147	2
1	C	3190	0	3237	168	0
2	B	576	0	586	28	0
2	D	571	0	575	26	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	1	0
3	D	1	0	0	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	1	0
5	A	108	0	0	3	0
5	B	18	0	0	1	0
5	C	135	0	0	5	0
5	D	17	0	0	0	0
All	All	8029	0	7824	364	2

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 23.

The worst 5 of 364 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:C:121:THR:HG22	1:C:124:ARG:NH1	1.21	1.48
1:A:263:SER:O	1:A:266:LYS:HG2	1.16	1.28
1:C:63:ASN:ND2	1:C:256[B]:CYS:SG	2.08	1.27
1:C:121:THR:CG2	1:C:124:ARG:NH1	1.99	1.23
1:C:121:THR:CG2	1:C:124:ARG:HH12	1.53	1.19

All (2) 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:77:LYS:NZ	1:A:135:ASP:OD1[7_554]	1.63	0.57
1:A:22:GLY:O	1:A:190:PRO:O[7_554]	2.10	0.10

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	425/446 (95%)	387 (91%)	31 (7%)	7 (2%)	7 6
1	C	392/446 (88%)	365 (93%)	21 (5%)	6 (2%)	8 7
2	B	68/88 (77%)	63 (93%)	5 (7%)	0	100 100
2	D	67/88 (76%)	62 (92%)	4 (6%)	1 (2%)	8 7
All	All	952/1068 (89%)	877 (92%)	61 (6%)	14 (2%)	8 7

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	83	SER
1	A	141	ILE
1	C	106	GLU
2	D	25	GLY

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	365/380 (96%)	338 (93%)	27 (7%)	13	14
1	C	346/380 (91%)	321 (93%)	25 (7%)	13	14
2	B	66/80 (82%)	63 (96%)	3 (4%)	24	32
2	D	65/80 (81%)	55 (85%)	10 (15%)	2	2
All	All	842/920 (92%)	777 (92%)	65 (8%)	12	13

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	31	LEU
2	D	35	ILE
1	A	393	SER
1	A	339	VAL
2	D	37	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	417	ASN
1	C	51	ASN
2	D	23	GLN
1	C	241	ASN
1	A	357	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 17 ligands modelled in this entry, 17 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	161:LEU	C	162:ARG	N	0.90

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	431/446 (96%)	0.92	77 (17%) 3 4	25, 44, 87, 115	0
1	C	401/446 (89%)	0.83	56 (13%) 6 7	22, 43, 87, 114	3 (0%)
2	B	71/88 (80%)	0.59	7 (9%) 13 14	29, 42, 67, 83	1 (1%)
2	D	71/88 (80%)	0.78	9 (12%) 8 9	30, 45, 72, 82	0
All	All	974/1068 (91%)	0.85	149 (15%) 5 6	22, 43, 85, 115	4 (0%)

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	ALA	11.7
1	A	116	ALA	9.3
1	A	265	VAL	9.2
1	A	117	TRP	7.6
1	A	358	ALA	7.3

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(\AA^2)	Q<0.9
4	CL	C	1443	1/1	0.89	0.24	72,72,72,72	0
4	CL	A	1441	1/1	0.91	0.23	70,70,70,70	0
4	CL	D	1089	1/1	0.91	0.21	63,63,63,63	0
4	CL	B	1088	1/1	0.93	0.16	53,53,53,53	0
4	CL	B	1089	1/1	0.93	0.20	73,73,73,73	0
3	HG	C	1439	1/1	0.94	0.23	55,55,55,55	1
4	CL	D	1088	1/1	0.95	0.23	66,66,66,66	0
4	CL	A	1442	1/1	0.95	0.20	58,58,58,58	0
4	CL	C	1441	1/1	0.96	0.26	57,57,57,57	0
3	HG	A	1438	1/1	0.96	0.14	78,78,78,78	1
4	CL	A	1440	1/1	0.97	0.15	68,68,68,68	0
3	HG	B	1087	1/1	0.97	0.09	77,77,77,77	1
4	CL	C	1442	1/1	0.97	0.24	66,66,66,66	0
3	HG	C	1438	1/1	0.98	0.10	78,78,78,78	1
3	HG	D	1087	1/1	0.98	0.08	69,69,69,69	1
3	HG	C	1440	1/1	0.99	0.14	40,40,40,40	1
3	HG	A	1439	1/1	0.99	0.14	45,45,45,45	1

6.5 Other polymers [i](#)

There are no such residues in this entry.